Symmetry and Group Theory

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Lecture – 14
Dipole Moment and Optical Activity

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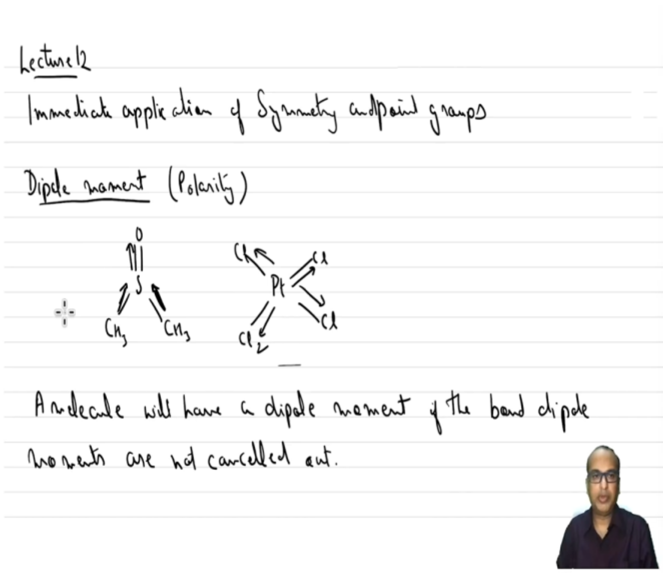

Welcome back everyone, so let us start lecture 12. So far, we have discussed symmetry present in the molecules and we have learned how to identify or how to classify the molecules based on the symmetry elements and symmetry operations present into various symmetry point groups. So, by now we should be well-versed with all the symmetry point groups, how to classify a molecule into different symmetry point groups, like, for example look at any object around yourself and or look at any take any molecule and try to classify into one of those symmetry point groups.

So that should be very very clear. So, once we have achieved that status, so we are ready to actually go for very first application which is let us say immediate application of symmetry point groups. So, the first property that we can predict or those we can identify or determine whether molecule has that physical property or not is dipole moment. So, we are all aware what is a dipole moment? So, dipole moment or polarity whether a molecule is polar or non-polar so whether a molecule is non-polar or polar it depends on whether a molecule has dipole moment or not.

So what is dipole moment? It is the separation of charges along any particular bond and let us say if all such separation of charges or all such bond moments add up together or not cancel against each other than the molecule is set to have that has a dipole moment. So, for example if we consider let us say some molecule just an example. So, in this case the dipole moment along this and this bond and along this bond is not going to cancel with each other whereas if we look at a molecule like this PtCl4.

The dipole moment along this side versus along this side will cancel against you to that similarly here it will cancel with this. So, this one will not have any net dipole moment or any molecule in such a metric may not have dipole moment but this molecule will have a dipole moment, so this molecule will be called as polar molecule and this will be called as non-polar molecule. So let us see with the rules of symmetry and point groups can we identify whether a molecule has dipole moment or not. So just to define a molecule.

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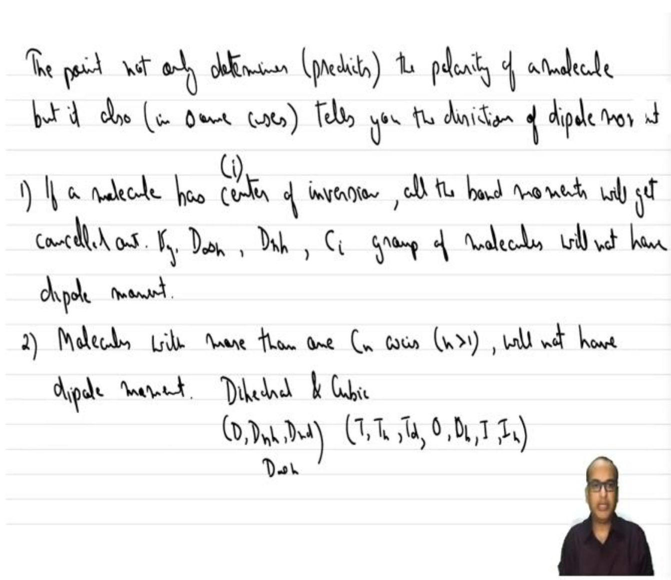

So, the point group not only determines, it does not only determines or predicts we can say, whether a molecule has dipole moment or not but in certain cases it will also tell you the direction of the dipole moment. So that is pretty interesting, I mean based on symmetry and based on the point groups you are able to predict whether a molecule has dipole moment or not and then you can also tell the direction of the dipole moment.

So, let us look at certain rules. So, we can say if a molecule has center of inversion all the bond moments will get canceled out. So, any point group that has i will not have dipole moment. So, what are the point groups we are left with. In such cases D-infinity-h, and Dnh, and what else Ci group of molecules these are examples certain examples, group of molecules will not have dipole moments.

So, why dipole moment is important? Because it tells you about the solubility of the molecule and then other certain other properties which depend on this dipole moment. So, it is important to know when you are doing chemistry it is important to know whether a molecule is polar or non-polar. So, molecules, with the same logic, molecules with more than one Cn axis with n greater than 1 will not have dipole moment. So that because if there are multiple more than one Cn axis it will cancel out the dipole moment of individual bonds.

So, this leaves the point groups let us say so all D point groups, dihedral point groups because they have Cn and n C2s perpendicular, so dihedral and cubic point groups, so this includes D, Dnh, Dnd, D-infinity-h and cubic means T, Th, Td, O, Oh, I, Ih. All these have more than one Cn axis so they will not have dipole moments. So that leaves a very few sets, so let us go ahead and see.

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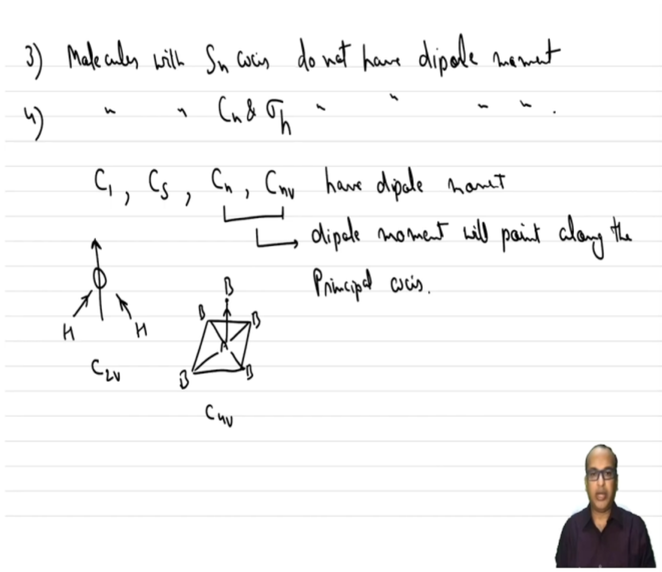

What else we are left with? So molecules with Sn axis that is improper rotation of rotation axis or we can also say Cn and sigma-h because if you have Cn and sigma-h then you will also have Sn vice versa is not true. So, we can say that molecules with Sn axis or let us make this as a separate point actually. So that it is not confusing, so molecules with Sn axis do not have dipole moments and now molecule with Cn and sigma-h do not have dipole moment.

So that leaves with what all point groups that will have dipole moment, one is C1 which does not have anything basically other than E, then Cs which will just have a plane of symmetry, Cn, and Cnv, these are the 4 point groups which have a dipole moment. So, life is very easy. Now if you want to know whether a dipole moment is there a molecule has dipole moment or not, all you have to do is just identify the point group.

If the molecule belongs to any of these 4, point groups it will have a dipole moment otherwise it will not. Also, in these 2 cases the dipole moment direction can be identified. It will point along the principal axis. So, because Cn and Cnv have only one Cn axis, only one principal axis there, only one rotation axis is there. So that will be the axis where the dipole moment will lie. So, we can take one example of this Cnv.

Which is let us say water molecule, the dipole moment will lie along the side which is very obviously because if you take the vector some of this dipole moment and this dipole moment it will lie along this side. So, it is a simple vector some dipole moments. Now similarly if you take a square pyramidal molecule, let us say something like this which is A, B, B, B. So, in this case the dipole moment will lie along this AB bond.

Because all the individual dipole moments will add up and will lie along the C4 axis, which is present. So, this is a C4v point group and this is C2v point group both of them belong to the Cnv and dipole moment will lie along the principal axis which is C4 in this case and C2 in this case. So this dipole moment concept should be very, very simple and straightforward wherever it is canceled of course it will not have but then it will be now directed by these set of point groups.

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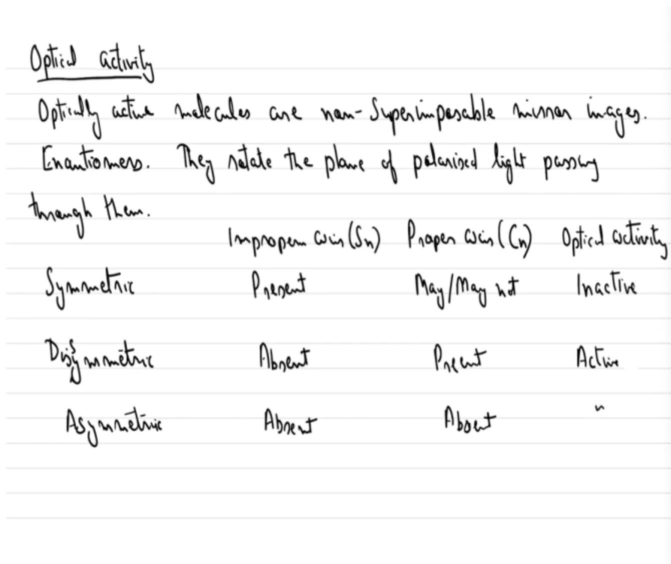

So, now let us look at the second important property which is called as optical activity. So again, optical activity is also important because for example racemic mixture of certain molecules are not active whereas only one particular optically active or one particular enantiomer is active in certain activities, for example many drug molecules racemic mixture is toxic but a particular enantiomer is actually active.

So, identifying optical activity is very very important when you are doing any kind of synthesis or any kind of chemistry and having to know optical activity based on symmetry is really helpful. So, what is optical activity is? Optical activity is the or we can say that optically active molecules are non superimposeble mirror images. So, if you take a molecule and if you take a mirror image of that.

And if you try to superimpose it when the molecules are non-superimposable you call it as optically active. What do you mean by optically active? and these are also called as enantiomers. So, the meaning of optical activity is that they rotate the plane of polarized light passing through them. So, you must have all done polarimeter experiment in your first year. I mean where you have taken sucrose solution.

And find out what is the optical rotation of that particular sucrose solution and do it as a function of concentration. So, there you must have seen that the plane of the polarized light is rotating. So that is because the sucrose is optically active. So, I am not going to go into details of how it is done. So, this is too basic for this course. So, you must know what is the meaning of plane polarized light and how it is rotated and also let us not go into that but our aim is to now identify on the basis of symmetry how a particular molecule can be identified whether it is optically active or not?

So, to understand this we should know the basic meaning of what is when a molecule is called as symmetric, when it is called as dissymmetric, and when it is called as asymmetric. So, we first test the presence or absence of improper axis, and then we test the presence or absence of proper axis. So symmetric molecules will have improper axis present and proper axis may or may not present, and optical activity, they are inactive.

So symmetric molecules which have Sn axis, so we can say this is Sn this is Cn. Now dissymmetric molecules Sn axis is absent and Cn axis is present, and they are optically active. Asymmetric molecules Sn is absent Cn also absent and they are also active.

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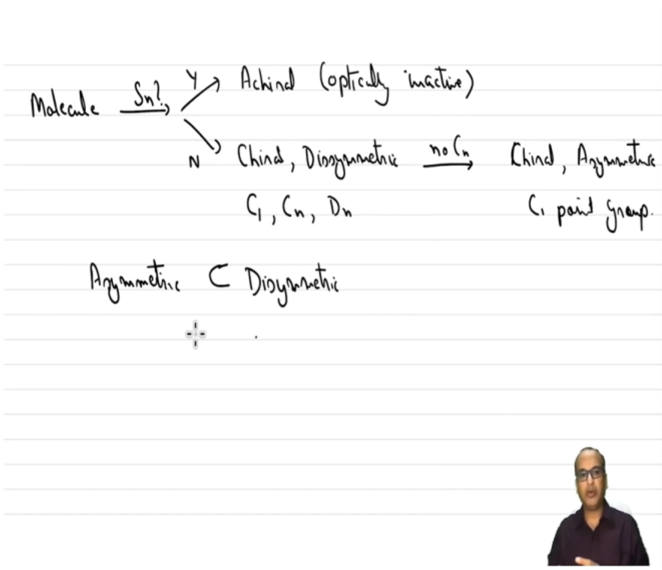

Or other way to identify this is let us say if you have a molecule and you are asking whether a Sn axis is present or not you will get 2 answers. So, I am trying to write a flowchart, yes or no. So, if Sn is present, then you assign it as Achiral. Achiral is optically inactive. And if a Sn is not present then you call it as chiral dissymmetric. Now what are the point groups to which this category belongs this will be C1, Cn, you can verify this and Dn.

Now if there is no Cn that will take these two out, and this will be called as chiral asymmetric and this will be C1 point group. So, we can say that asymmetric molecules are actually subset of dissymmetric molecules. So vice versa is not true say asymmetric is a subset of dissymmetric molecule, so all is asymmetric molecules are dissymmetric but all dissymmetric molecules are not asymmetric but they are all chiral.

So that sums up the optical activity and the dipole moment. So, you know now if a molecule is having one of these point groups, then it will be optically active and then if a molecule is having one of these 4, point groups and the molecule will have dipole moment. So, based on point group classification, you can identify at least 2 physical properties of the molecule which is a big deal in itself. So that finishes our discussion on symmetry and point groups.

And now we will see how symmetry properties are utilized using the concepts of group theory into more details into more applications. So, let us finish this lecture here today and then we will look into group theory details from now on. So, from now on it will be assumed that given a molecule you know how to identify the point group. So that portion will not be discussed if a molecule is now taken to discuss any details of group theory.

So, we will not be discussing what is the point group, how that particular molecule is classified into that particular point group. So, we will be only discussing straightaway classifying that molecule as this point group and then from there the discussion will start. So, I am trying to separate these 2 topics, so that you know that this is the symmetry topic and now we will move to group theory which will be more application oriented and then we will develop the theory part of the group theory part how symmetry properties of molecules will be utilized in group theory. So, let us finish this discussion today and thank you.